Heptanedinitrile

Other names:	1,5-Dicyanopentane
	PENTAMETHYLENE DICYANIDE
	PIMELIC ACID DINITRILE
	PIMELONITRILE
Inchi:	InChI=1S/C7H10N2/c8-6-4-2-1-3-5-7-9/h1-5H2
InchiKey:	LLEVMYXEJUDBTA-UHFFFAOYSA-N
Formula:	C7H10N2
SMILES:	N#CCCCCCC#N
Mol. weight [g/mol]:	122.17
CAS:	646-20-8

Physical Properties

Property code	Value	Unit	Source
gf	274.42	kJ/mol	Joback Method
hf	141.95	kJ/mol	Joback Method
hfus	15.02	kJ/mol	Fusion and solid-to-solid transitions of a homologous series of alkane-a,w-dinitriles
hvap	52.13	kJ/mol	Joback Method
log10ws	-2.49		Crippen Method
logp	1.984		Crippen Method
mcvol	112.250	ml/mol	McGowan Method
pc	2657.03	kPa	Joback Method
tb	563.72	K	Joback Method
tc	768.64	K	Joback Method
tf	298.63	K	Joback Method
vc	0.479	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	250.95	J/mol×K	563.72	Joback Method
cpg	259.69	J/mol×K	597.87	Joback Method
cpg	267.99	J/mol×K	632.03	Joback Method

cpg	275.87	J/mol×K	666.18	Joback Method
cpg	283.33	J/mol×K	700.33	Joback Method
cpg	290.40	J/mol×K	734.49	Joback Method
cpg	297.09	J/mol×K	768.64	Joback Method
hfust	15.00	kJ/mol	241.70	NIST Webbook
hvapt	74.50	kJ/mol	318.50	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	448.70	K	1.90	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	1.64050e+02
Coeff. B	-1.46677e+04
Coeff. C	-2.20521e+01
Coeff. D	2.02482e-05
Temperature range (K), min.	306.15
Temperature range (K), max.	330.15

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
KDB:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1420
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Temperature Dependence of the Relative Static Permittivity of Homologous Series of Liquid 1,n-Dicyanoalkanes N=C (CH2)n C=N, n = 2 to 8.	https://www.doi.org/10.1021/je300958c
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1420
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C646208&Units=SI
Fusion and solid-to-solid transitions of a homologous series of alkane-a,w-dinitriles:	https://www.doi.org/10.1016/j.jct.2007.03.005

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume